Hexadecanal

Other names: 1-Hexadecanal
Palmitaldehyde
n-Hexadecanal
Inchi: InChI=1S/C16H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h16H,2-15H2,1H3
InchiKey: NIOYUNMRJMEDGI-UHFFFAOYSA-N
Formula: C16H32O
SMILES: CCCCCCCCCCCCCCCC=O
Mol. weight [g/mol]: 240.42
CAS: 629-80-1

Physical Properties

Property code	Value	Unit	Source
gf	-15.68	kJ/mol	Joback Method
hf	-459.15	kJ/mol	Joback Method
hfus	39.48	kJ/mol	Joback Method
hvap	89.70	kJ/mol	NIST Webbook
log10ws	-5.80		Crippen Method
logp	5.667		Crippen Method
mcvol	237.870	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1811.00		NIST Webbook
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rinpol	1796.00	NIST Webbook
rinpol	1761.00	NIST Webbook
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rinpol	1817.00	NIST Webbook
rinpol	1817.00	NIST Webbook
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rinpol	1821.00	NIST Webbook
rinpol	1794.00	NIST Webbook
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ripol	2098.00		NIST Webbook
ripol	2120.00		NIST Webbook
ripol	2154.00		NIST Webbook
ripol	2119.00		NIST Webbook
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ripol	2135.00		NIST Webbook
ripol	2135.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2119.00		NIST Webbook
ripol	2132.00		NIST Webbook
ripol	2146.00		NIST Webbook
ripol	2153.00		NIST Webbook
ripol	2153.00		NIST Webbook
ripol	2154.00		NIST Webbook
ripol	2164.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2141.00		NIST Webbook
ripol	2123.00		NIST Webbook
ripol	2120.00		NIST Webbook
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ripol	2137.00		NIST Webbook
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ripol	2154.00		NIST Webbook
ripol	2108.00		NIST Webbook
ripol	2121.00		NIST Webbook
ripol	2124.00		NIST Webbook
tb	614.14	K	Joback Method
tc	778.10	K	Joback Method
tf	308.00 ± 4.00	K	NIST Webbook
tf	303.00 ± 8.00	K	NIST Webbook
tf	307.00 ± 3.00	K	NIST Webbook
tf	320.00 ± 4.00	K	NIST Webbook
tf	331.70 ± 20.00	K	NIST Webbook
tf	309.00 ± 4.00	K	NIST Webbook
tf	307.00 ± 3.00	K	NIST Webbook
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.69	J/mol×K	778.10	Joback Method
cpg	726.34	J/mol×K	750.77	Joback Method
cpg	711.33	J/mol×K	723.45	Joback Method
cpg	695.64	J/mol×K	696.12	Joback Method
cpg	679.25	J/mol×K	668.79	Joback Method
cpg	662.13	J/mol×K	641.47	Joback Method
cpg	644.27	J/mol×K	614.14	Joback Method
dvisc	0.0040946	Pa×s	312.08	Joback Method
dvisc	0.0001725	Pa×s	614.14	Joback Method
dvisc	0.0002310	Pa×s	563.80	Joback Method
dvisc	0.0003276	Pa×s	513.45	Joback Method
dvisc	0.0005014	Pa×s	463.11	Joback Method
dvisc	0.0008512	Pa×s	412.77	Joback Method
dvisc	0.0016739	Pa×s	362.42	Joback Method
hvapt	67.60	kJ/mol	494.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	474.20	K	3.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50033e+01
Coeff. B	-5.09569e+03
Coeff. C	-1.03544e+02
Temperature range (K), min.	449.82
Temperature range (K), max.	629.32

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629801&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume